TIME-SERIES PREDICTION USING CONSTRAINED FORMULATION FOR NEURAL NETWORK TRAINING AND CROSS VALIDATION

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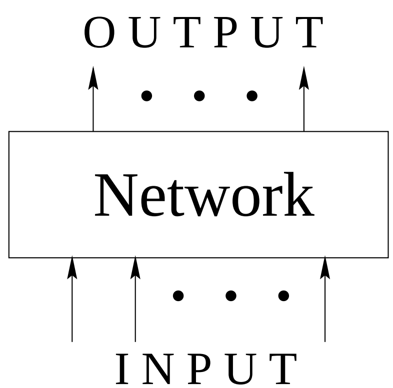
Outline

- **Motivations**
- **Constrained formulations for artificial neural-network (ANN) training**
- **Training algorithms for constrained formulation**
  - Discrete Lagrange-multiplier theory (DLM)
  - Constrained simulated annealing (CSA)
  - Integration of back-propagation and CSA
- **Experimental results**
- **Conclusions**

ANN Model for Time-Series Prediction

- Time-series prediction
  - Given a sequence of values observed in the past, predict future values
- ANN model for time-series
  - Feedforward
  - Weights adjustment



Traditional Formulations for ANN Training

- Unconstrained formulation

$$\min_{w} \quad E(w) = \sum_{t=1}^{n} ||\vec{o}_t(w) - \vec{d}_t||^2, \tag{1}$$

- Training algorithms
  - BP/BP variants and gradient-based methods
  - Genetic algorithms
  - Simulated annealing
- Issues
  - No guidance when search reaches a local minimum of $E(w)$
  - Nonuniform errors on patterns – not best for prediction

Traditional Cross-Validation

- Divide historical data into two disjoint sets
  - Training set
  - Cross-validation set
- Issues
  - Hard to choose appropriate validation set: where and how long?
  - Data used for cross-validation cannot be used for training
  - Only one validation set is used at any time: not good when time series is multi-stationary

Motivations

- Motivations
  - Unconstrained formulation leads to either poor solution quality or long training time
  - Multiple cross-validation sets are needed for multi-stationary time-series
  - Unsatisfied pattern may provide extra guidance for further search
  - Our previous successful application of constrained formulation
    - * Two-spiral problem: 4 hidden units with only 19 weights
- Proposed solution
  - Use constrained formulation for ANN training and cross validation
  - Solve constrained problem using constrained simulated annealing

Performance Metrics

- One output unit
- Normalized mean square error (nMSE)

$$\varepsilon = \frac{1}{\sigma^2 N} \sum_{t=t_0}^{t_1} (y(t) - d(t))^2, \qquad (2)$$

  - σ^2 is the variance of the true time series in $[t_0, t_1]$
  - $y(t)$ is the actual output, $d(t)$ is the desired output
  - N is number of patterns in the measurement

- Open-loop single-step measurement: external input is true observed data
- Close-loop iterative measurement: external input is predicted output obtained in the last iteration

Proposed Constrained Formulation

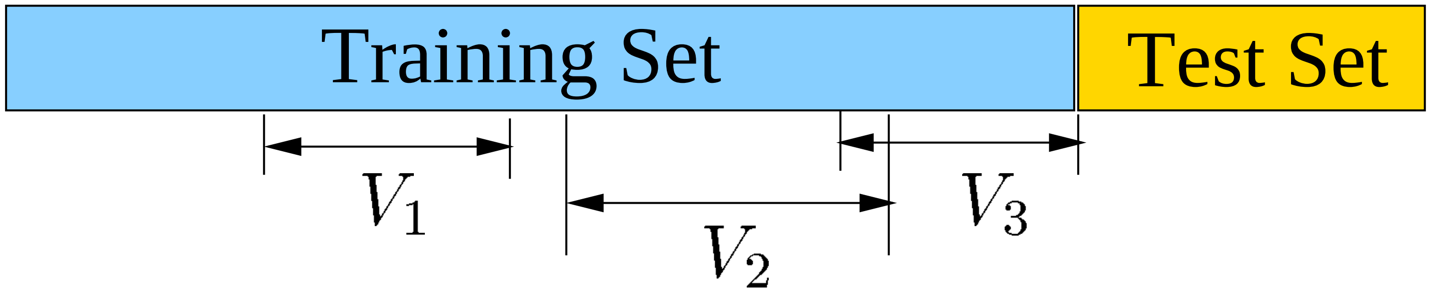
- Each pattern treated as an additional constraint
- Constrained formulation

$$\begin{aligned} \min_w \; & E(w) = \sum_{t=1}^{n} max^2\{|o_t(w) - d_t| - \tau, 0\} \\ \text{s.t.} \; & h_t(w) = |o_t(w) - d_t| \le \tau, \end{aligned} \quad (3)$$

  - τ decreases towards 0 as looser constraints are satisfied
  - Equivalent to unconstrained formulation when $\tau = 0$
- Advantages
  - Unsatisfied constraints provide extra guidance when search reaches a sub-optimum of the objective function
  - Introduction of τ allows even training for all patterns: important when there is no solution to $E(w) = 0$

Proposed Cross-Validation Method

- Multiple validation set(s) within training set
- Iterative and single-step validation errors added as new constraints
- Advantages
  - Training patterns fully used
  - Multiple validation sets cover multiple regimes in a multi-stationary time series
  - Flexibility in choosing validation sets – location and length



Constrained Formulation with Cross Validation

- Constrained formulation

$$
\begin{array}{lll}
\min_w & E(w) = \sum_{t=1}^{n} max^2\{|o_t(w) - d_t| - \tau, 0\} & \\
\text{s.t.} & h_t(w) = |o_t(w) - d_t| \leq \tau & (4) \\
 & h_i^I(w) = \varepsilon_i^I \leq \tau_i^I & \\
 & h_i^S(w) = \varepsilon_i^S \leq \tau_i^S, &
\end{array}
$$

  - ε_i^I: nMSE of iterative validation error on the i^{th} validation set
  - ε_i^S: nMSE of single-step validation error on the i^{th} validation set
  - τ_i^I and τ_i^S: small positive values and refined successively as training progresses

- Constrained formulation solved by *constrained simulated annealing* (CSA) which is based on *discrete Lagrange-multiplier theory*

Discrete Lagrange-Multiplier Theory

- Discrete equality-constrained *nonlinear programming problem* (NLP):

$$\begin{aligned} \text{minimize}_x \quad & f(x) \\ \text{subject to} \quad & h(x) = 0, \end{aligned} \tag{5}$$

where $x = (x_1, \cdots, x_n)$ is discrete.

- Inequality constraint transformation: $g_j(x) < 0 \Longrightarrow max(g_j(x), 0) = 0$
- Generalized discrete augmented Lagrangian function of (5):

$$L_d(x, \lambda) = f(x) + \lambda^T H\left(h(x)\right) + \frac{1}{2}||h(x)||^2, \tag{6}$$

where H is a non-negative transformation

- $Neighborhood$ $\mathcal{N}(x)$ of x
  - *Finite* user-defined set of discrete points that satisfy reachability

Discrete Lagrange-Multiplier Theory (cont'd)

- *Saddle point* (SP_{dn}) $(x^\star, \lambda^\star)$

$$L_d(x^*, \lambda) \le L_d(x^*, \lambda^*) \le L_d(x, \lambda^*) \tag{7}$$

  for all $x \in \mathcal{N}(x^*)$ and all $\lambda \in R$.

- *Constrained local minimum* (CLM_{dn}):
  - Feasible and $f(x') \ge f(x)$ for all $x' \in \mathcal{N}(x)$
- *Constrained global minimum* (CGM_{dn}):
  - Feasible and $f(x') \ge f(x)$ for all x' in search space
- First-order necessary and sufficient conditions for CLM_{dn}
  - One-to-one correspondence between CLM_{dn} and SP_{dn}

Constrained Simulated Annealing (CSA)

- Look for discrete-space saddle points by doing descents in free-variable w space and ascents in Lagrange-multiplier space
- Converge to CGM_{dn} under certain conditions

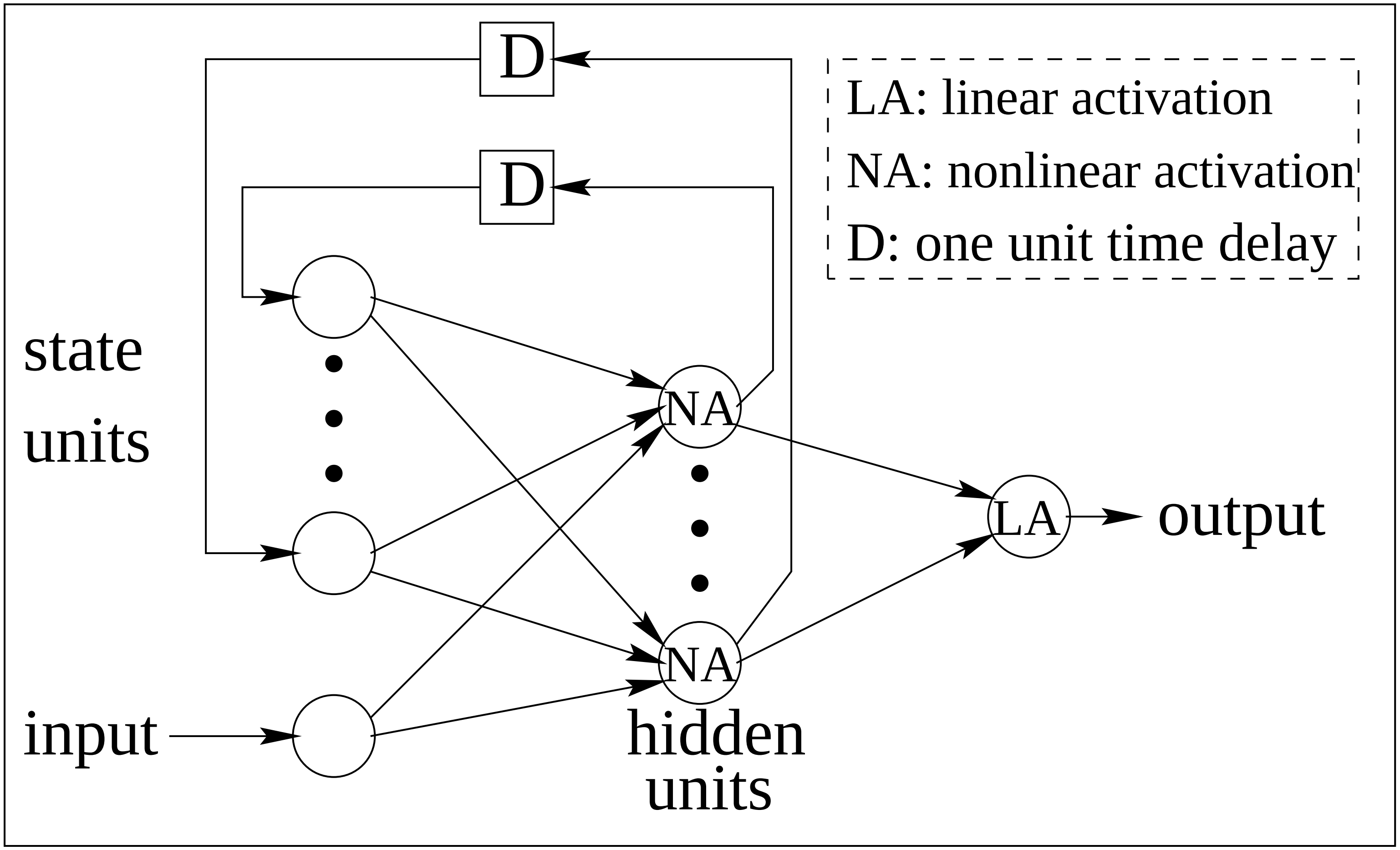
procedure CSA
    set initial $\mathbf{x} = (x, \lambda)$ by randomly generating x and by setting $\lambda \leftarrow 0$;
    initialize starting temperature T to be large enough and the cooling rate $0 < \alpha < 1$
    set N_T (number of trials per temperature);
    while stopping condition is not satisfied **do**
        for $n \leftarrow 1$ **to** N_T **do**
            generate $\mathbf{x}'$ from $\mathcal{N}(\mathbf{x})$ using $G(\mathbf{x}, \mathbf{x}')$;
            accept $\mathbf{x}'$ with probability $A_T(\mathbf{x}, \mathbf{x}')$
        end_for
        reduce temperature by $T \leftarrow \alpha \times T$;
    end_while
end_procedure

Integration of Back-Propagation and CSA

- Random sampling too expensive
  - Use epoch-wise back-propagation through time (EWBPTT)
- Integration of EWBPTT into CSA to generate new try point $w + \delta w$

Architecture in Use

- Recurrent ANN: 1 input unit, n hidden units, and 1 output unit



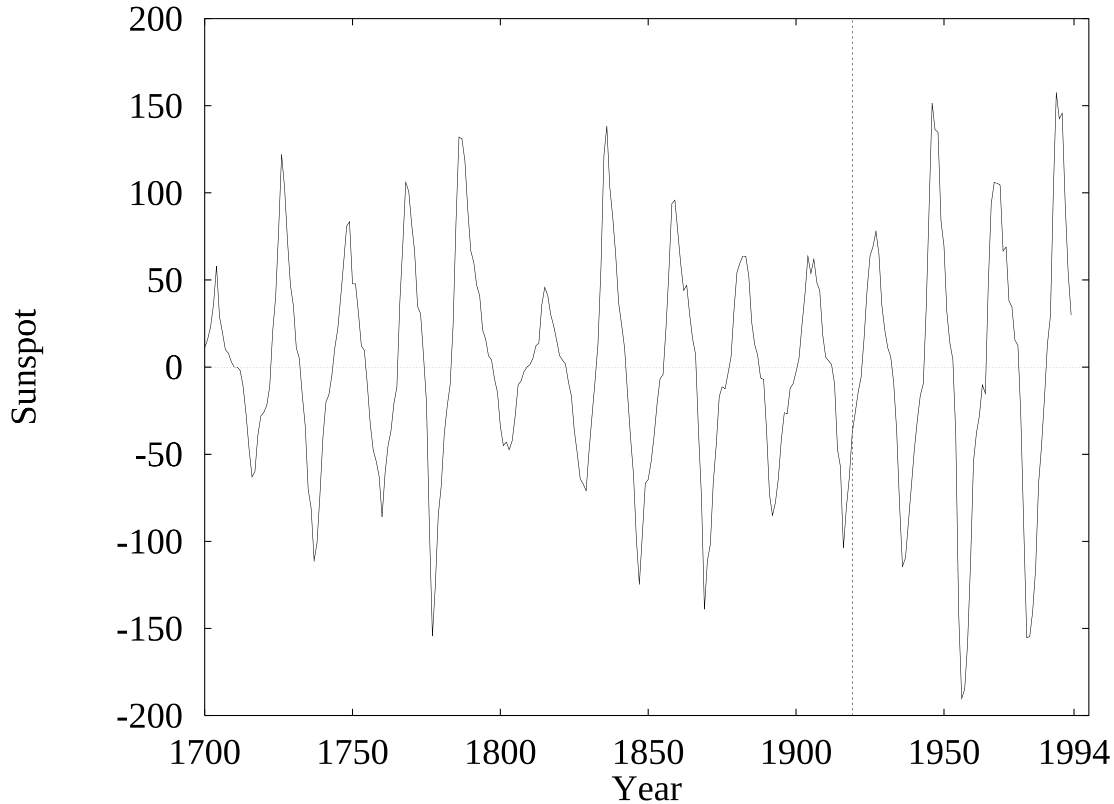
Comparisons of 5 Training Methods

SA:	Unconstrained,	SA,	No cross-validation
SA&V1:	Unconstrained,	SA,	Traditional cross-validation
CSA:	Constrained,	CSA,	No cross-validation
CSA&V1:	Constrained,	CSA,	Traditional cross-validation
CSA&V2:	Constrained,	CSA,	Proposed cross-validation

Test Data:

- Sunspot time series: yearly number of sun-spots (1700-1994)
  - Training data: 1700-1920
  - Testing data: 1921-1994
  - Cross-validation data: 1900-1921

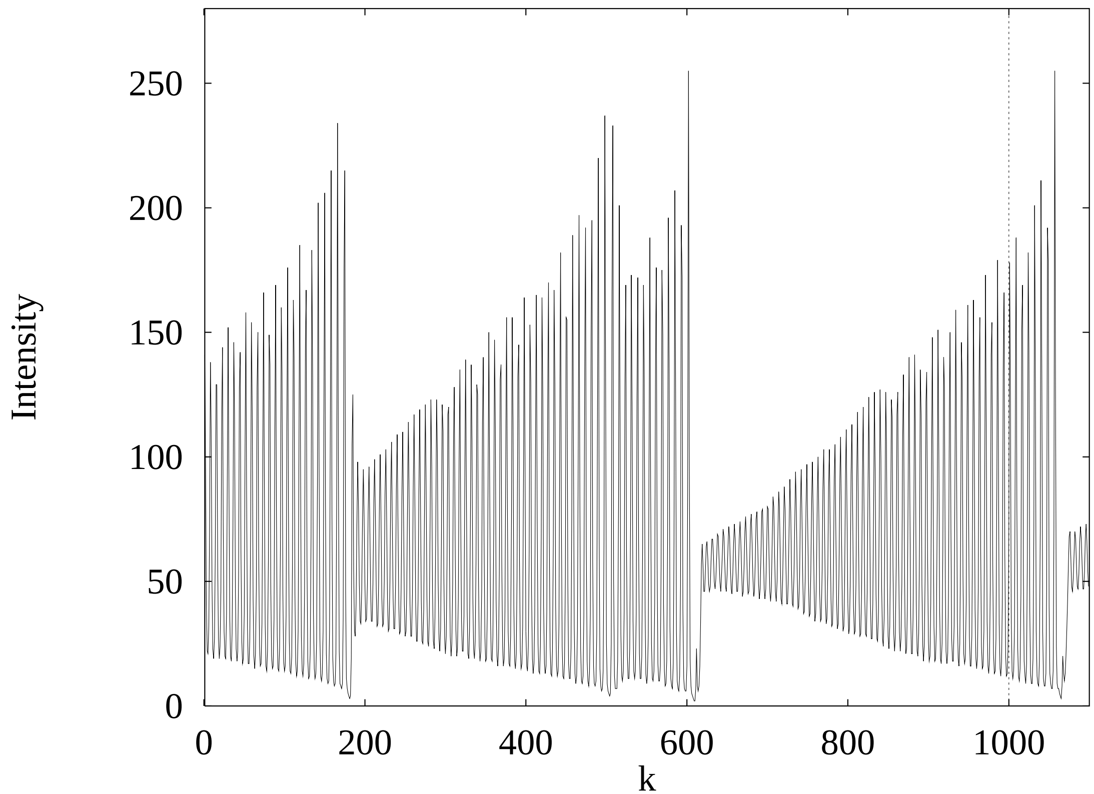
Sunspots Time Series



Dotted vertical line separates training set and test set

- ANN used: 1 input, 2 hidden units, 1 output – 11 weights in total

Laser Time Series



Dotted vertical line separates training set and test set

- Laser time-series: 1 input – 20 hidden units – 1 output, 461 weights

Results on Sunspots

- 24 to 26 seconds per run on a 450MHz P III with Solaris 2.7

Average prediction nMSE (with 95% confidence on $\pm 10\%$)

Method	1921-1955	1956-1979	1980-1994	1921-1994	Runs
SA	0.052306	0.113958	0.055074	0.076735	28
SA&V1	0.081943	0.138510	0.086798	0.102199	76
CSA	0.035385	0.061361	0.039559	0.045554	10
CSA&V1	0.042079	0.086607	0.051244	0.060784	18
CSA&V2	0.034288	0.053549	0.034236	0.040634	4

- Observations:
  - Without cross-validation, CSA consistently out-performs SA
  - Traditional cross-validation does not work well
  - CSA&V2 out-performs all other algorithms and is the most stable

Comparison with Previous Work on Sunspots

Method	No. of Free Variables	Training	Single-Step Testing			
		1700-1920	1921-55	1956-79	1980-94	1921-94
AR(12)	14	0.128	0.126	0.36	0.306	0.238
TAR	18	0.097	0.097	0.28	0.306	0.197
WNet	113	0.082	0.086	0.35	0.313	0.219
SSNet	N/A	-	0.077	N/A	N/A	N/A
DRNN	30	0.105	0.091	0.273	N/A	N/A
COMM	N/A	0.079	0.065	0.24	0.188	0.148
ScaleNet	N/A	0.086	0.057	0.13	N/A	N/A
Proposed CSA&V2	11	0.0559	0.0337	0.0524	0.0332	0.0397

AR(12): 12^{th}-order linear auto-regression

TAR: Threshold auto-regressive model

WNet: Feedforward ANN with weight elimination

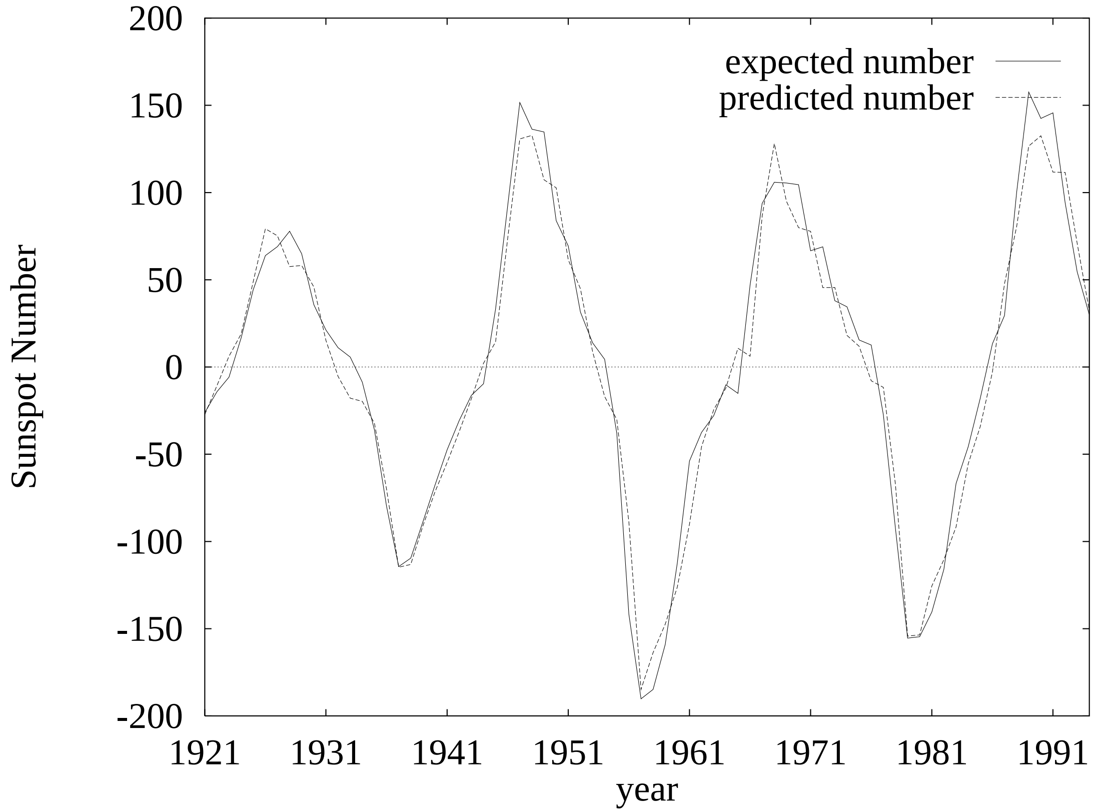
SSNet:Soft-weight-sharing network

DRNN: Dynamic recurrent ANN

COMM: Committee prediction using FIR network

ScaleNet: Multiscale ANN

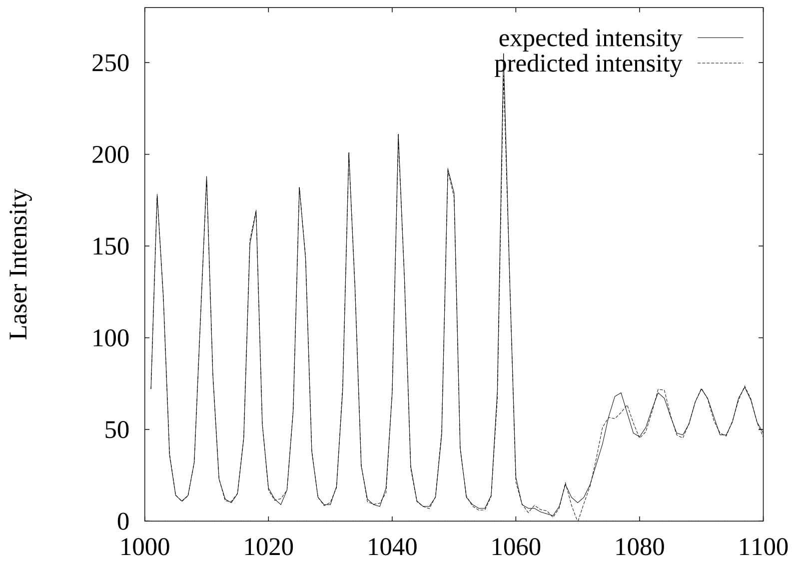
Single-step Prediction for Sunspots



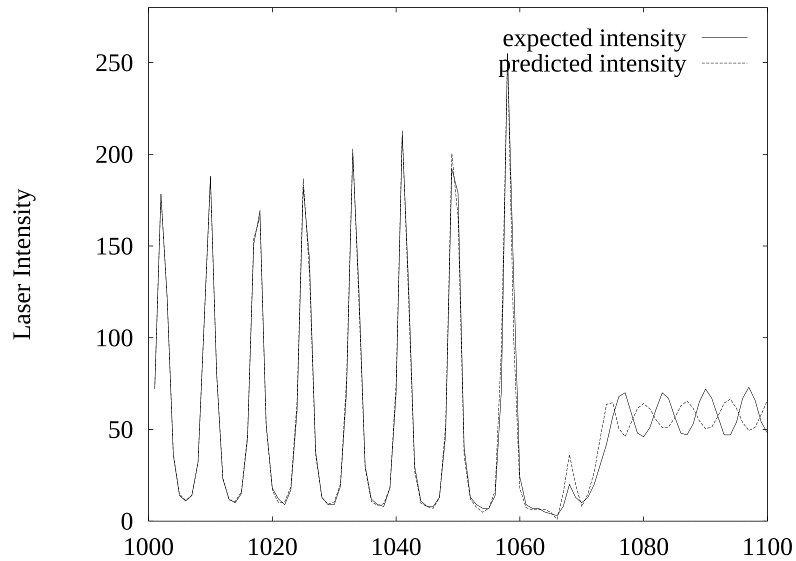
Comparisons with Previous Work on Laser

Method	Number of weights	Training	Single Step Prediction		Iterative Prediction	
		100-1000	1001-1050	1001-1100	1001-1050	1001-1100
FIR network	1105	0.00044	0.00061	0.023	0.0032	0.0434
ScaleNet	N/A	0.00074	0.00437	0.0035	N/A	N/A
CSA&V2 (Run 1)	461	0.00036	0.00043	0.0034	0.0054	0.0194
CSA&V2 (Run 2)	461	0.00107	0.00030	0.00276	0.0030	0.0294

Predictions for Laser Time-Series



Single-step prediction



Iterative prediction

Conclusions

- Constrained formulation with proposed cross-validation method CSA$V2 is effective, stable, and out-performs previous work significantly on two benchmarks
- Future work
  - Improve speed and solution quality of training algorithm
  - Study non-stationary time-series: stock and currency exchange time-series